Interfacial Thermal Transport in Diamond: Insights from Simulation

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Diamond has the highest thermal conductivity of any known material. The effect of interfaces on the thermal conductivity is of considerable interest for applications in diamond nanostructures. We use large-scale molecular-dynamics simulations to determine the thermal conductances of a number of representative grain boundaries in diamond. We compare these with the thermal conductances in the corresponding grain boundaries in Si. We ascribe the differences between the results for diamond and silicon to the very different thermal conductivities in the bulk and to the differences in the structures of the interfaces. The implications of our results on the possibility of using nanocrystalline and ultra-nanocrystalline diamond for thermal transport applications are discussed.